ALCF Early Science Program

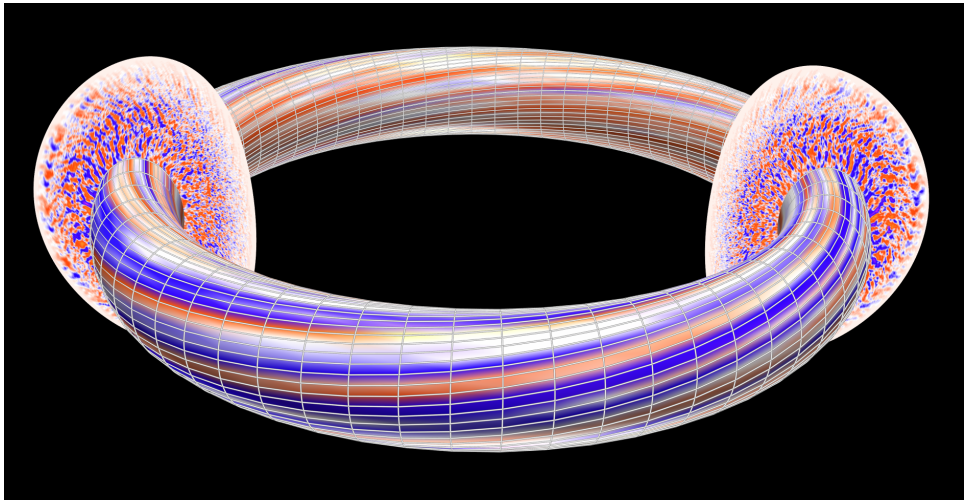
Argonne NATIONAL LABORATORY

ESP Kick-Off Workshop
Project Plan Presentation

Global Simulation of Plasma Microturbulence at the Petascale & Beyond

PI: William Tang (PPPL)

Presenter: Tim Williams (ANL)



October 18-19, 2010

Project Overview

Kinetic simulation of turbulent energy transport in magnetic fusion devices

- **GTC-P**
  - Large-aspect-ratio equilibrium magnetic geometry
    - Circular cross-section
- **GTS**
  - Extreme D-shape cross sections of existing tokamak fusion devices
    - Initial magnetic equilibrium set from experimental parameters
- **Mira enables physical ITER scale simulations previously not possible on Intrepid**
- **Validated simulations & associated understanding of gyro-Bohm confinement would be major milestone for ITER**
    - ***Insensitivity to increased system size (ITER-scale) associated with Gyro-Bohm confinement is a major advantage over unfavorable Bohm-like scaling observed in most present-generation tokamaks***

Scientific Field: Fusion

Codes: GTS, GTC-P

Computational Approach, Numerical Methods

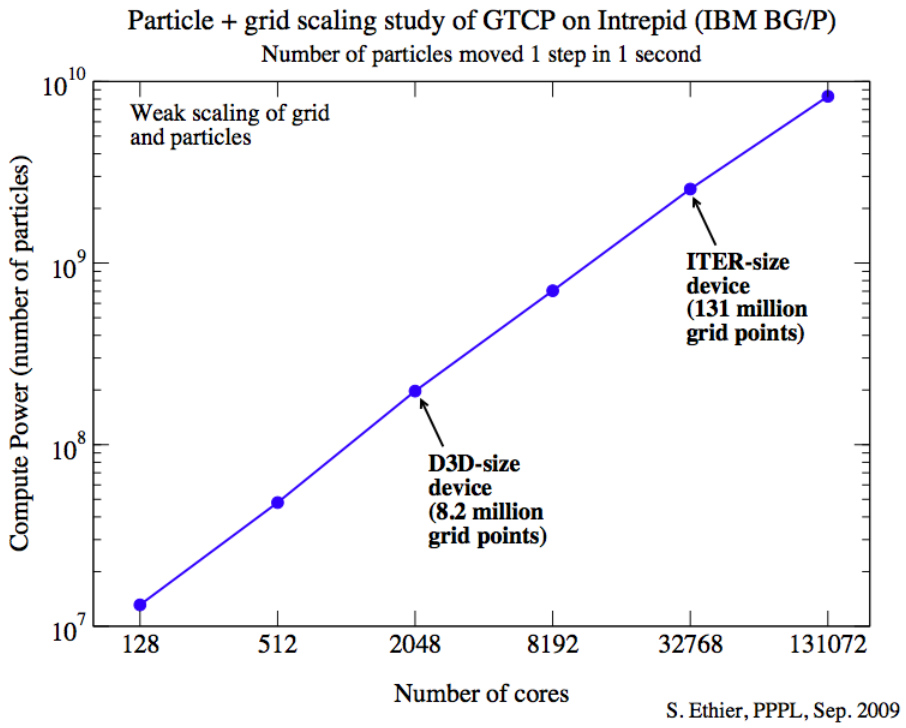
- ***Gyrokinetic* plasma description efficient for microturbulence regime**
  - Solve gyrophase-averaged Vlasov-Poisson
  - Removes the fast cyclotronic time scale while keeping all non-local effects of gyration (particles are charged rings)
- **Particle-in-cell plasma simulation**
  - Charge of discrete simulation particles deposited to grid
  - Self-consistent (electrostatic) field from solution of Poisson equation
    - PETSc solver (GMRES + Newton pre-conditioner)
  - Particles move under force interpolated from field
  - GTC-P: adiabatic electrons
  - GTS: full electron dynamics

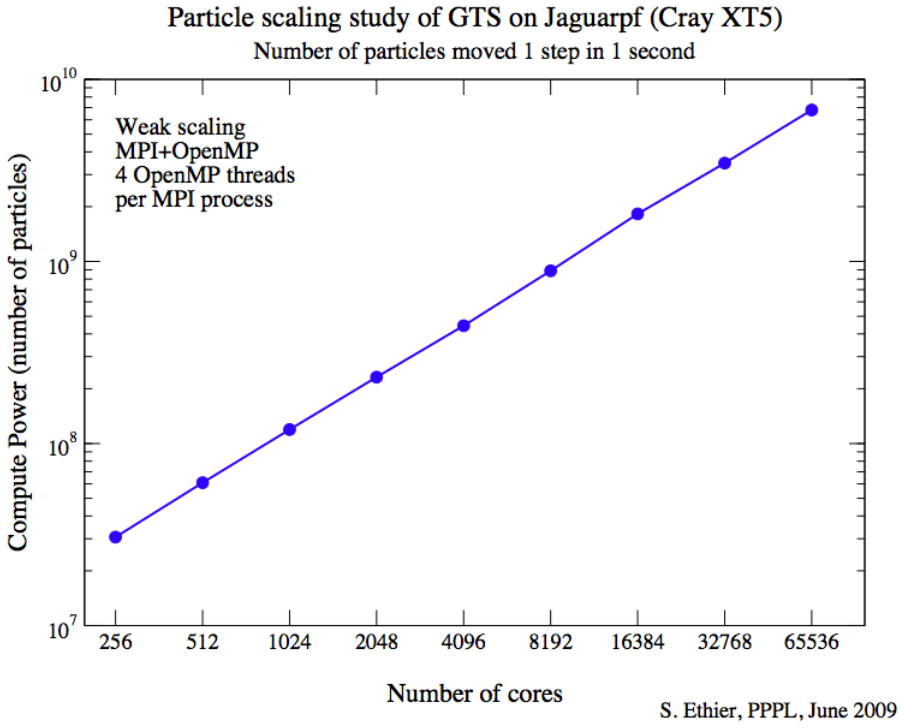
Parallelism and Existing Implementation

- **MPI parallelism:**
  - 1D domain decomposition in toroidal direction (long way around)
  - GTS: Particles distributed within subdomain
  - GTC-P: 2nd dimension domain decomposition (radial)
- **OpenMP parallelism**
  - Loop-level directives
- **I/O: ADIOS**
  - Only for checkpoint-restart at the moment

Parallelism and Existing Implementation (2)

- **Current Performance/Scalability**





Library and Tool Dependencies

- **Libraries**
  - PETSc (solver for Poisson equation)
  - ADIOS (parallel I/O)
  - SPRNG 2.0 (random number generators)
  - PSPLINE (spline and hermite interpolation tools)
- **Tools**
  - VisIt

Anticipated Modifications for Blue Gene/Q

- **Node-level parallelism**
  - Increase ratio of OpenMP parallelism to MPI processes
- **Processor-specific optimization at core level**
- **Port GTC-P optimizations to GTS**
  - 2D domain decomposition
- **Performance and scaling needed to run proposed problem on Mira:**
  - ITER minor radius 4x current experiments such as DIII-D
    - 600 million grid cells
    - 50 billion particles
  - Need O(4x) speed of Intrepid for reasonable wallclock turnaround
    - Scale out to Intrepid cores = 640,000 Mira cores
      - About 320,000 Mira cores

Plan for Next 6 Months Effort

- **Help find and hire a project postdoc**
- **On Intrepid:**
  - Measure GTC-P performance w.r.t. increased OpenMP and decreased MPI
    - Project to estimate Mira performance
    - Simultaneously start work on optimizing multithread charge accumulation
  - Diagnose GTC-P load imbalance beyond 32K cores
    - Need to balance grid work (radial decomposition) with particle work
    - Manifested in local force calculation
  - Port GTC-P optimizations to GTS